Research Article

Heisenberg Uncertainty Relation in Quantum Liouville Equation

Davide Valenti

Gruppo di Fisica Interdisciplinare, Dipartimento di Fisica e Tecnologie Relative, Università di Palermo and INFM-CNR, Unità di Palermo, Viale delle Scienze, Ed. 18, I-90128 Palermo, Italy

Correspondence should be addressed to Davide Valenti, valentid@gip.dft.unipa.it

We consider the quantum Liouville equation and give a characterization of the solutions which satisfy the Heisenberg uncertainty relation. We analyze three cases. Initially we consider a particular solution of the quantum Liouville equation: the Wigner transform $f(\mathbf{x},\mathbf{v},t)$ of a generic solution $\psi(\mathbf{x};t)$ of the Schrödinger equation. We give a representation of $\psi(\mathbf{x}, t)$ by the Hermite functions. We show that the values of the variances of $\mathbf{x}$ and $\mathbf{v}$ calculated by using the Wigner function $f(\mathbf{x},\mathbf{v},t)$ coincide, respectively, with the variances of position operator $\widehat{X}$ and conjugate momentum operator $\widehat{P}$ obtained using the wave function $\psi(\mathbf{x},t)$. Then we consider the Fourier transform of the density matrix $\rho(\mathbf{z},\mathbf{y},t) = \psi^*(\mathbf{z},t)\psi(\mathbf{y},t)$. We find again that the variances of $\mathbf{x}$ and $\mathbf{v}$ obtained by using $\rho(\mathbf{z}, \mathbf{y},t)$ are respectively equal to the variances of $\widehat{X}$ and $\widehat{P}$ calculated in $\psi(\mathbf{x},t)$. Finally we introduce the matrix $\|A_{nn'}(t)\|$ and we show that a generic square-integrable function $g(\mathbf{x},\mathbf{v},t)$ can be written as Fourier transform of a density matrix, provided that the matrix $\|A_{nn'}(t)\|$ is diagonalizable.

1. Introduction

In nonrelativistic quantum mechanics the state of a system formed by N particles is described by a state vector whose x-representation is given by the wave function $\psi(\mathbf{x}, t)$ ($\mathbf{x}$ is the generic vector of a $3N$-dimensional space). The square modulus of $\psi(\mathbf{x}, t)$ represents the probability density that the particle is found in $\mathbf{x}$ at the time t. The time evolution of the state vector (or, more precisely, the evolution of the corresponding wave function) is given by the Schrödinger equation [1]

$$
\imath\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta_{\mathbf{x}}\psi(\mathbf{x},t) + V(\mathbf{x},t)\psi(\mathbf{x},t). \tag{1.1}
$$

In classical mechanics the dynamics of a system is described by the Newton's equations of motion which represent trajectory equations. Alternatively Lagrange or Hamilton formulations emphasize other concepts, for example, the law of energy conservation, but essentially nothing different is introduced [2].

A system formed by N particles, for example, a gas, is usually studied by the tools of the statistical mechanics and its state may be described instantaneously by a probability function which depends on both positions and velocities of the particles [3, 4]. The time evolution of a statistical system can be obtained by several different equations. In particular a system formed by N particles in a potential $V(\mathbf{x}, t)$ can be described by the classic Liouville equation [5]

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{v}} f = 0. \tag{1.2}$$

The function $f(\mathbf{x}, \mathbf{v}, t)$ is a probability density and it instantaneously describes the system state inside the $6N$-dimensional phase space $\{\mathbf{x}, \mathbf{v}\}$. The use of the Liouville equation instead of Newton's equations shifts the emphasis from the concept of trajectory to that of probability.

When the time evolution of a many-particle system is considered, it is useful to obtain single-particle approximation of the classic Liouville equation. The Vlasov limit [6], where the field is scaled as $1/N$ for particles' number approaching infinite, and the use of a one-dimensional model allow to obtain an equation which is formally identical to (1.2), the classic Liouville equation in a two-dimensional phase space

$$\frac{\partial f(x, v, t)}{\partial t} + v \frac{\partial f(x, v, t)}{\partial x} - \frac{\partial V(x, t)}{\partial x} \frac{\partial f(x, v, t)}{\partial v} = 0. \tag{1.3}$$

In these conditions the probability function describes the density of single particle in an unitary segment. In general, the *Vlasov equation* [7, 8] provides the probability density of finding a single particle at the position $\mathbf{x}$ with speed $\mathbf{v}$ at the time t ($\mathbf{x}$ and $\mathbf{v}$ are vectors belonging to the ordinary three-dimensional space). The use of the statistical mechanics allows to connect the mechanical properties (mycroscopical domain) of the constituting particles with the thermodynamic behaviour (macroscopical domain) of the system. Moreover the importance of a formulation of classical mechanics based on the Liouville equation is that quantum mechanics may be introduced from classical mechanics amended by suitable postulates and principles [9].

In quantum physics a system can be also described by using the tools of the statistical mechanics. The use of a stochastic formulation to describe the exciton transport in polar media [10] and the existence of relation connecting physical observables with the temperature [11] emphasize the importance of introducing statistical tools to resolve typical problems of the quantum physics. It is useful to remember that ultimately in solid state physics the study of the dressing processes of excitons and conduction electrons in polar media [12–16] has been accompanied by the realization of experimental techniques allowing to create excitons within times of the order of hundred femtoseconds [17, 18]. When one deals with dressing processes in the matter, the use of the statistical mechanics allows to treat a many-particle system as an ensemble. This leads to a thermodynamic-like description of quantum phenomena [19–21]. In example, the dressing dynamics of excitons and polarons

may be connected with some mean properties of the matter and the theoretical results may be compared with the experimental observations [22–25].

The statistical treatment of a quantum system may be led by introducing an equation describing the global behaviour of the system and simultaneously considering that it undergoes the laws of the quantum physics. In particular, it is possible to obtain an equation which represents the extension of the Liouville equation to the quantum mechanics. For sake of semplicity the particle system will be described referring to the Vlasov equation (i.e., the Liouville equation for $N = 1$). A one-dimensional model will be studied without loss of generality. Considerations and results can be successively extended to the multiparticle case. For $N = 1$ the one-dimensional Schrödinger equation is

$$\imath\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x,t)\psi(x,t). \tag{1.4}$$

Defining the density matrix

$$\rho(z,y,t) = \psi^*(z,t)\psi(y,t), \tag{1.5}$$

where ψ^* represents the conjugate complex of ψ, from Schrödinger equation (1.4) one obtains

$$\imath\hbar\frac{\partial\rho}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\rho}{\partial y^2} + \frac{\hbar^2}{2m}\frac{\partial^2\rho}{\partial z^2} - V(z)\rho + V(y)\rho. \tag{1.6}$$

Setting

$$z = x + \frac{\hbar}{2m}s, \qquad y = x - \frac{\hbar}{2m}s, \tag{1.7}$$

$$u(x,s,t) = \rho\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s, t\right), \tag{1.8}$$

(1.6) becomes

$$\frac{\partial u}{\partial t} + \imath\frac{\partial}{\partial s}\left(\frac{\partial u}{\partial x}\right) - \imath\frac{V(x + (\hbar/2m)s, t) - V(x - (\hbar/2m)s, t)}{\hbar}u = 0. \tag{1.9}$$

Now the Wigner distribution function may be introduced [26]

$$f = \frac{1}{2\pi}\int_{R_s} u(x,s,t)e^{\imath s v}ds. \tag{1.10}$$

From (1.9) the one-dimensional *quantum Liouville equation* [5] is obtained

$$\frac{\partial f(x,v,t)}{\partial t} + v\frac{\partial f(x,v,t)}{\partial x} + Wf = 0 \tag{1.11}$$

with

$$Wf = -i\frac{1}{2\pi}\int_{R_s}\int_{R_{v'}}\frac{V(x+(\hbar/2m)s,t)-V(x-(\hbar/2m)s,t)}{\hbar}$$
$$\cdot f(x,v',t)e^{is(v-v')}dv'ds.$$

(1.12)

The term $-(\partial V(x,t)/\partial x)(\partial f(x,v,t)/\partial v)$ in the classic Liouville equation (1.3) is replaced in the quantum extension (1.11) by the term Wf. The linear operator W is named pseudodifferential operator and it is applied by a product operation acting on the Fourier transform f. The multiplicator $\widehat{W}$, that is, the symbol of the pseudodifferential operator, is obtained comparing (1.9) and (1.11)

$$\widehat{W} = -i\frac{V(x+(\hbar/2m)s,t)-V(x-(\hbar/2m)s,t)}{\hbar}.$$

(1.13)

Using the Liouville equation in the place of Schrödinger equation allows to deal with statistical mixtures of states which cannot be represented by a wave function. These states may be defined by considering a complete set of orthonormal solutions for the Schrödinger equation ψ_j $(j = 1, 2, \ldots)$: a state is obtained as a mixture, with probabilities $\lambda_j (0 \le \lambda_j \le 1; \sum_j \lambda_j = 1)$, of the orthonormal solutions. The corresponding density matrix is given by

$$\rho(z,y,t) = \sum_j \lambda_j \psi_j^*(z,t)\psi_j(y,t) = \sum_j \lambda_j \rho_j(z,y,t),$$

(1.14)

where $\rho_j(z,y,t)$ is the density matrix of the quantum state represented by the wave function ψ_j (pure case). Since $\rho(z,y,t)$ is a linear combination of solutions of (1.6), it is a solution of the same equation. Defining u and f as in (1.8) and (1.10) we observe that generally the quantum Liouville equation allows to describe statistical mixture of states (nonpure case).

Moreover the use of tools of statistical mechanics in treating quantum problems allows to consider the effects due to the continuous reduction of the spatial domains where the solid state physics works. The dimensions of the modern semiconductor devices become comparable with the free mean path of the electrons which can cross the active zone without undergoing scattering processes. These problems can be overcrossed by considering the distribution function of the electrons $f(x,v,t)$ and by introducing equations typical of the statistical mechanics whose solutions provide a more precise and correct description of the dynamics of these systems [27, 28]. Yet, the increasing reduction of the dimensions where these devices work does not allow to neglect the quantum effects. It is necessary to use equations including these contributions by extending the classical models to the quantum physics [29]. Then, knowing the mathematical characteristics of these equations becomes very important in order to study the physical properties of the systems considered. Particularly, it was shown that the quantum hydrodynamic equation directly obtained from the Schrödinger equation have solutions which generally do not converge to the corresponding classical solutions, when the Planck constant tends to zero [30]. This problem can be overcrossed by introducing the Wigner transform and the quantum Liouville equation given respectively by (1.10) and (1.11). In fact, it was shown that for $\hbar \to 0$ the solutions of the quantum Liouville equation converge to those of the corresponding classical equation

[31, 32]. Yet, the use of the quantum Liouville equation to describe a quantum system suggests the necessity of verifying that this equation satisfies the Heisenberg uncertainty relation. In this paper we give a characterization of the solutions of the quantum Liouville equation (QLE) which satisfy the Heisenberg uncertainty relation. At this aim we show that for suitable conditions the variances Δx and Δv calculated by using a solution of the QLE coincide identically with the variances $\Delta\widehat{X}$ and $\Delta\widehat{P}$ of position operator and conjugate momentum operator obtained by using the corresponding Schrödinger solution $\psi(x,t)$.

2. Square-Integrable Functions $\psi(X,T)$: The Space L^2

Any arbitrary solution $\psi(x)$ of the Schrödinger equation, due to its expandibility in plane waves,

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\, \overline{\psi}(k)\, e^{\imath k x},\tag{2.1}$$

verifies the inequality[1]

$$\Delta\widehat{X}\,\Delta\widehat{P} \geq \frac{\hbar}{2},\tag{2.2}$$

where $\widehat{X}$ and $\widehat{P}$ are observables which satisfy the commutation rule

$$\left[\widehat{X},\widehat{P}\right] = \imath\hbar.\tag{2.3}$$

The probabilistic interpretation [33, 34] of the wave function $\psi(x,t)$ of a particle implies that $|\psi(x,t)|^2 dx$ is the probability of measuring, at the time t, the particle inside a segment with amplitude dx and centered in x (one-dimensional model). The total probability of detecting the particle somewhere in space has to be obviously equal to 1 (probability conservation), so we must have

$$\int_{-\infty}^{+\infty} dx\, |\psi(x,t)|^2 = 1.\tag{2.4}$$

With each pair of square-integrable functions $\phi(x,t)$, $\psi(x,t)$ a complex number is associated by the definition of *scalar product*

$$(\phi,\psi) = \int_{-\infty}^{+\infty} dx\, \phi^*(x)\, \psi(x).\tag{2.5}$$

The set of the square-integrable functions conjunctly with the correspondence defined in (2.5) is called L^2 and it has the structure of a Hilbert space [35–37]. L^2 satisfies all the criteria of a vector space where the scalar product is given by the operation defined in (2.5). From a physical point of view the set L^2 is too wide. It is then useful to reduce the set of square-integrable functions to the ones which possess certain properties of regularity and

describe real physical systems. The functions have to be everywhere defined, (a probability value must be associated to the particle at every point in the space); the functions must be everywhere continuous (the probability amplitude in an arbitrary point of the space x_0 cannot depend on the size of the volume which contains the particle); the functions have to be infinitely differentiable (this also assures the possibility of approximating them by a Taylor's expansion). No complete list of the necessary properties is given; the prescription is only considering in L^2 the set F constituted by functions which are "enough" regular, that is functions which are suitable for describing the behavior of real physical systems.

As we said in the previous sections, the dynamics of a quantum system can be described applying the formalism of the statistic mechanics. This treatment can be performed by using the *quantum Liouville equation* introduced in the first section. In order to obtain the QLE, the passage from the density matrix $\rho(x + (\hbar/2m)s, x - (\hbar/2m)s, t)$ as a function of x and s to the Wigner function $f(x, v, t)$ has been performed. It is not obvious that the variances Δx and Δv, obtained using the Wigner functions $f(x, v, t)$, satisfy the Heisenberg uncertainty relation. In the following, a study of the solutions of the quantum Liouville equation is performed. A solution of the quantum Liouville equation is obtained considering the Wigner transform $f(x, v, t)$ of an arbitrary Schrödinger function $\psi(x, t)$ (pure state). Expanding $\psi(x, t)$ by Hermite functions, it is shown that the variances of x and v obtained using the Wigner function $f(x, v, t)$ coincide respectively with the variances of the operators position and conjugate momentum calculated using the wave function $\psi(x, t)$.

This comparison is repeated exploiting a more general solution, that is the Fourier transform of an arbitrary density matrix (Wigner function for a statistical mixture of states). The results show that any solution of the quantum Liouville equation, defined as Fourier transform of any density matrix, also verifies the Heisenberg uncertainty relation.

Finally a larger characterization is presented for functions which contemporaneously satisfy both the quantum Liouville equation and the Heisenberg relation. This characterization is obtained by defining the space S^2 of the square-integrable functions. We show that the Heisenberg inequality is verified by an arbitrary function $f(x, v, t) \in S^2$ provided that, given any arbitrary basis $\{T_{nn'}(x, v)\}$ in S^2, the matrix $\|A_{nn'}(t)\|$ of the coefficients of the expansion

$$f(x, v, t) = \sum_{nn'} A_{nn'}(t) T_{nn'}(x, v) \tag{2.6}$$

is diagonalizable.

3. Heisenberg Relation and Wigner Distribution Function: Pure State

The "enough" regular solutions of the Schrödinger equation which belong to the space F, verify instantaneously the Heisenberg uncertainty relation

$$\Delta \widehat{X} \Delta \widehat{P} \geq \frac{\hbar}{2}, \tag{3.1}$$

where $\widehat{X}$ and $\widehat{P}$ are observables which satisfy the commutation rule [1]

$$\left[\widehat{X}, \widehat{P}\right] = \imath \hbar. \tag{3.2}$$

In x representation $\widehat{X}$ and $\widehat{P}$ coincide respectively with the operator which multiplies by x and with the differential operator $(\hbar/i)(\partial/\partial x)$.

In order to characterize the solutions of the quantum Liouville equation which preserves the Heisenberg relation, we calculate the variances Δx and Δv using the Wigner transform of a generic solution $\psi(x,t)$ of the one-dimensional Schrödinger equation (1.4). For this purpose we introduce the basis composed of the Hermite functions. Consider an arbitrary solution of (1.4) (Schrödinger equation) and its Wigner transform given by (1.10) (pure state case). It is known that the Hermite functions, which are defined by

$$S_n = \left(\frac{1}{\pi}\right)^{1/4} e^{-x^2/2} \frac{1}{\sqrt{2^n n!}} H_n(x), \tag{3.3}$$

where $H_n(x)$ is the Hermite polynomial of degree n given by [38, 39]

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}, \tag{3.4}$$

constitute a basis in F.

We may expand the generic wave function $\psi(x,t)$ on this basis obtaining

$$\psi(x,t) = \left(\frac{1}{\pi}\right)^{1/4} e^{-x^2/2} \sum_n \frac{A_n(t)}{\sqrt{2^n n!}} H_n(x) \tag{3.5}$$

with $A_n(t)$ given by

$$A_n(t) = \int_{R_x} dx\, \psi^*(x,t) S_n(x). \tag{3.6}$$

For the mean values of X and X^2 it results

$$\langle X \rangle = \int_{R_x} dx\, \psi^*(x,t) x \psi(x,t), \tag{3.7}$$

$$\left\langle X^2 \right\rangle = \int_{R_x} dx\, \psi^*(x,t) x^2 \psi(x,t). \tag{3.8}$$

The integrals present in (3.7) and (3.8) may be worked out by means of the expansion of $\psi(x,t)$ in Hermite functions. By using (3.5) and (3.7) the expression for $\langle X \rangle$ becomes

$$\langle X \rangle = \left(\frac{1}{\pi}\right)^{\frac{1}{2}} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^{n'} n'! 2^n n!}} \int_{-\infty}^{+\infty} dx\, x\, e^{-x^2} H_n(x) H_{n'}(x). \tag{3.9}$$

Analogously, by using (3.5) in (3.8), one obtains

$$\langle X^2 \rangle = \left(\frac{1}{\pi}\right)^{1/2} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^{n'} n'! 2^n n!}} \int_{-\infty}^{+\infty} dx \, x^2 \, e^{-x^2} H_n(x) H_{n'}(x). \tag{3.10}$$

For the mean value of $\widehat{P}$ it results

$$\langle \widehat{P} \rangle = \frac{\hbar}{i} \left(\frac{1}{\pi}\right)^{1/2} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^{n'} n'! 2^n n!}}$$

$$\cdot \left[n' \int_{-\infty}^{+\infty} dx \, e^{-x^2} H_n(x) H_{n'-1}(x) - n \int_{-\infty}^{+\infty} dx \, e^{-x^2} H_{n'}(x) H_{n-1}(x) \right]. \tag{3.11}$$

Finally, by using (3.5), for the mean value of $\widehat{P}^2$ we get

$$\langle \widehat{P}^2 \rangle = -\hbar^2 \left(\frac{1}{\pi}\right)^{1/2} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^{n'} n'! 2^n n!}} \cdot$$

$$\cdot \left[-\frac{1}{2} \int_{-\infty}^{+\infty} dx \, e^{-x^2} H_n(x) H_n'(x) - 2nn' \int_{-\infty}^{+\infty} dx \, e^{-x^2} H_{n-1}(x) H_{n'-1}(x) \right.$$

$$\left. + n(n-1) \int_{-\infty}^{+\infty} dx \, e^{-x^2} H_{n-2}(x) H_n'(x) + n'(n'-1) \int_{-\infty}^{+\infty} dx \, e^{-x^2} H_{n'-2}(x) H_n(x) \right]. \tag{3.12}$$

In order to show that the variances $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ and $\Delta v = \sqrt{\langle v^2 \rangle - \langle v \rangle^2}$ verify the Heisenberg uncertainty relation, we may compare them with the variances $\Delta \widehat{X} = \sqrt{\langle \widehat{X}^2 \rangle - \langle \widehat{X} \rangle^2}$ and $\Delta \widehat{P} = \sqrt{\langle \widehat{P}^2 \rangle - \langle \widehat{P} \rangle^2}$ of the operators $\widehat{X}$ and $\widehat{P}$ calculated by using the wave function $\psi(x,t)$. It is then necessary to calculate the mean values $\langle x \rangle$, $\langle x^2 \rangle$, $\langle v \rangle$, $\langle v^2 \rangle$ using the formalism of Wigner transform. By using the expansion given in (3.5), the Wigner transform (1.10) of the generic wave function $\psi(x,t)$ becomes (setting $m = 1$)

$$f = \frac{1}{2\pi} \sum_n \sum_{n'} \left(\frac{1}{\pi}\right)^{1/2} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^n n! 2^{n'} n'!}}$$

$$\cdot \int_{-\infty}^{+\infty} ds \, e^{isv} e^{-(x+(\hbar/2)s)^2/2} e^{-(x-(\hbar/2)s)^2/2} H_n\left(x + \frac{\hbar}{2}s\right) H_{n'}\left(x - \frac{\hbar}{2}s\right). \tag{3.13}$$

Now we may obtain the mean value of x, x^2, v, and v^2 using the distribution function given in (3.13). For $\langle x \rangle$ it results

$$\langle x \rangle = \left(\frac{1}{\pi}\right)^{1/2} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^n n! 2^{n'} n'!}} \int_{-\infty}^{+\infty} dx \, x e^{-x^2} H_n(x) H_{n'}(x). \tag{3.14}$$

By following an analogous procedure we obtain

$$\langle x^2 \rangle = \left(\frac{1}{\pi} \right)^{1/2} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^n n! 2^{n'} n'!}} \int_{-\infty}^{+\infty} dx \, x^2 e^{-x^2} H_n(x) H_{n'}(x). \tag{3.15}$$

In a similar way one obtains the expression giving the mean value of v

$$\langle v \rangle = i\hbar \sum_n \sum_{n'} \left(\frac{1}{\pi} \right)^{1/2} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^n n! 2^{n'} n'!}}$$
$$\cdot \int_{-\infty}^{+\infty} dx \, e^{-x^2} \left[n H_{n-1}(x) H_{n'}(x) - n' H_{n'-1}(x) H_n(x) \right]. \tag{3.16}$$

Finally the expression for the mean value of v^2 is obtained

$$\langle v^2 \rangle = -\hbar^2 \left(\frac{1}{\pi} \right)^{1/2} \sum_n \sum_{n'} \frac{A_n^*(t) A_{n'}(t)}{\sqrt{2^n n! 2^{n'} n'!}} \int_{-\infty}^{+\infty} dx \, e^{-x^2}$$
$$\cdot \left[-\frac{1}{2} H_n(x) H_{n'}(x) + n(n-1) H_{n-2}(x) H_{n'}(x) \right.$$
$$\left. + n'(n'-1) H_n(x) H_{n'-2}(x) - 2n \, n' H_{n-1}(x) H_{n'-1}(x) \right]. \tag{3.17}$$

The comparison between the set constituted by (3.9), (3.10), (3.11), (3.12) and that formed by (3.14), (3.15), (3.16), (3.17) indicates that the variances $\Delta \widehat{X}$ and $\Delta \widehat{P}$ of the quantum operators $\widehat{X}$ and $\widehat{P}$ calculated by the use of a generic wave function $\psi(x, t)$ coincide respectively with the variances Δx and Δv of the variables x and v obtained by using the Wigner transform $f(x, v, t)$ defined in (1.10).

4. Heisenberg Relation and Wigner Distribution Function: Statistical Mixture of States

Within the usual one-dimensional model we consider a quantum particle whose dynamics is given by the Liouville equation. The state of the particle is represented by the Wigner distribution function obtained as Fourier transform of the density matrix $\rho(x + (\hbar/2m)s, x - (\hbar/2m)s, t)$. In the most general case, as we said, the density matrix (and then the corresponding Wigner function) describes a statistical mixture of states which is not associated with a wave function. Using a basis of the space F, the density matrix of the system

can be expressed in terms of density matrices of pure states. For example, if $\{r_j\}$ is a basis of the vectorial space F, an arbitrary density matrix is given by

$$\rho\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s, t\right) = \sum_j \lambda_j r_j^*\left(x + \frac{\hbar}{2m}s\right)r_j\left(x - \frac{\hbar}{2m}s\right)$$

$$= \sum_j \lambda_j \rho_j\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s\right) \tag{4.1}$$

with

$$\rho_j\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s\right) = r_j^*\left(x + \frac{\hbar}{2m}s\right)r_j\left(x - \frac{\hbar}{2m}s\right). \tag{4.2}$$

The coefficients λ_j, which determine the time evolution of the system, satisfy the relation

$$\sum_j \lambda_j = 1. \tag{4.3}$$

Due to the presence of the single contributions ρ_j, (4.1) allows to introduce again the idea of wave function. Each of these contributions represents the density matrix of a pure state. The mean value of an arbitrary operator is then obtained using the Wigner distribution function calculated as Fourier transform of $\rho(x + (\hbar/2m)s, x - (\hbar/2m)s, t)$ and it can be expressed by the linear combination of the mean values calculated in each pure state

$$\langle x \rangle = \sum_j \lambda_j \langle x \rangle_j, \qquad \langle x^2 \rangle = \sum_j \lambda_j \langle x^2 \rangle_j,$$

$$\langle v \rangle = \sum_j \lambda_j \langle v \rangle_j, \qquad \langle v^2 \rangle = \sum_j \lambda_j \langle v^2 \rangle_j, \tag{4.4}$$

where $\langle \rangle_j$ represents the mean value obtained using the Wigner function

$$f_j(x, v, t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} ds\, e^{isv}\rho_j\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s\right). \tag{4.5}$$

We must evaluate if the product $\Delta x \Delta v$ satisfies the Heisenberg relation for every set of λ_j. We then consider a statistical mixture of N quantum states which is described, at the time t, by the density matrix given in (4.1). The corresponding Wigner function is given by

$$f(x, v, t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} ds\, e^{isv}\rho\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s, t\right)$$

$$= \frac{1}{2\pi}\sum_j \lambda_j \int_{-\infty}^{+\infty} ds\, e^{isv}\rho_j\left(x + \frac{\hbar}{2m}s, x - \frac{\hbar}{2m}s\right). \tag{4.6}$$

The mean square deviations of x and v calculated in $f(x, v, t)$ are given by

$$(\Delta x)^2 = \sum_j \lambda_j \left\langle x^2 \right\rangle_j - \sum_j \lambda_j^2 \langle x \rangle_j^2 - \sum_{i \neq j} \lambda_i \lambda_j \langle x \rangle_i \langle x \rangle_j, \tag{4.7}$$

$$(\Delta v)^2 = \sum_j \lambda_j \left\langle v^2 \right\rangle_j - \sum_j \lambda_j^2 \langle v \rangle_j^2 - \sum_{i \neq j} \lambda_i \lambda_j \langle v \rangle_i \langle v \rangle_j. \tag{4.8}$$

Note that (4.7) can be written

$$
\begin{aligned}
(\Delta x)^2 &= \sum_j \lambda_j \left(\left\langle x^2 \right\rangle_j - \lambda_j \langle x \rangle_j^2 \right) - \sum_{i \neq j} \lambda_i \lambda_j \langle x \rangle_i \langle x \rangle_j \\
&= \sum_j \lambda_j \left[(\Delta x_j)^2 + (1 - \lambda_j) \langle x \rangle_j^2 \right] - \sum_{i \neq j} \lambda_i \lambda_j \langle x \rangle_i \langle x \rangle_j \\
&= \sum_j \lambda_j (\Delta x_j)^2 + \sum_{i \neq j} \lambda_i \lambda_j \langle x \rangle_j^2 - \sum_{i \neq j} \lambda_i \lambda_j \langle x \rangle_i \langle x \rangle_j \\
&= \sum_j \lambda_j (\Delta x_j)^2 - \sum_{i < j} \lambda_i \lambda_j \left(\langle x \rangle_j - \langle x \rangle_i \right)^2.
\end{aligned}
\tag{4.9}
$$

By an analogous procedure, from (4.8) one gets

$$(\Delta v)^2 = \sum_j \lambda_j (\Delta v_j)^2 - \sum_{i < j} \lambda_i \lambda_j \left(\langle v \rangle_j - \langle v \rangle_i \right)^2. \tag{4.10}$$

Finally using (4.9) and (4.10) one gets

$$
\begin{aligned}
(\Delta x)^2 (\Delta v)^2 &= \sum_{j,j'} \lambda_j (\Delta x)_j^2 \lambda_{j'} (\Delta v)_{j'}^2 \\
&\quad + \sum_{i < j, j'} \lambda_i \lambda_j \left(\langle x \rangle_j - \langle x \rangle_i \right)^2 \lambda_{j'} (\Delta v)_{j'}^2 \\
&\quad + \sum_{j, i' < j'} \lambda_j (\Delta x)_j^2 \lambda_{i'} \lambda_{j'} \left(\langle v \rangle_j - \langle v \rangle_i \right)^2 \\
&\quad + \sum_{i < j, i' < j'} \lambda_i \lambda_j \left(\langle x \rangle_i - \langle x \rangle_j \right)^2 \lambda_{i'} \lambda_{j'} \left(\langle v \rangle_{i'} - \langle v \rangle_{j'} \right)^2.
\end{aligned}
\tag{4.11}
$$

Setting

$$\Theta = \sum_{i<j,j'} \lambda_i \lambda_j \left(\langle x \rangle_j - \langle x \rangle_i \right)^2 \lambda_{j'} (\Delta v)^2_{j'}$$

$$+ \sum_{j,i'<j'} \lambda_j (\Delta x)^2_j \lambda_{i'} \lambda_{j'} \left(\langle v \rangle_j - \langle v \rangle_i \right)^2$$

$$+ \sum_{i<j,i'<j'} \lambda_i \lambda_j \left(\langle x \rangle_i - \langle x \rangle_j \right)^2 \lambda_{i'} \lambda_{j'} \left(\langle v \rangle_{i'} - \langle v \rangle_{j'} \right)^2,$$

(4.12)

(4.11) becomes

$$(\Delta x)^2 (\Delta v)^2 = \sum_{j,j'} \lambda_j (\Delta x)^2_j \lambda_{j'} (\Delta v)^2_{j'} + \Theta.$$

(4.13)

From (4.13) it results

$$(\Delta x)^2 (\Delta v)^2 = \sum_{j'<j} \lambda_j \lambda_{j'} \left[(\Delta x)^2_j (\Delta v)^2_{j'} + (\Delta x)^2_{j'} (\Delta v)^2_j \right]$$

$$+ \sum_j \lambda^2_j (\Delta x)^2_j (\Delta v)^2_j + \Theta.$$

(4.14)

The term Θ is nonnegative. Moreover, as we showed in the previous section, the variances $(\Delta x)_j$ and $(\Delta v)_j$ obtained using Wigner transform of pure states coincide with the variances $(\Delta \widehat{X})_j$ and $(\Delta \widehat{P})_j$ calculated by the corresponding wave functions and they satisfy the Heisenberg uncertainty relation

$$(\Delta x)^2_j (\Delta v)^2_j \geq \frac{\hbar^2}{4} \implies (\Delta v)^2_j \geq \frac{\hbar^2}{4} \frac{1}{(\Delta x)^2_j}$$

(4.15)

which implies

$$(\Delta x)^2_{j'} (\Delta v)^2_j \geq \frac{\hbar^2}{4} \frac{(\Delta x)^2_{j'}}{(\Delta x)^2_j}.$$

(4.16)

Using (4.15) and (4.16) in (4.14) the following inequality is obtained:

$$(\Delta x)^2 (\Delta v)^2 \geq \frac{\hbar^2}{4} \sum_j \lambda^2_j + \frac{\hbar^2}{4} \sum_{j'<j} \lambda_j \lambda_{j'} \left[\frac{(\Delta x)^2_j}{(\Delta x)^2_{j'}} + \frac{(\Delta x)^2_{j'}}{(\Delta x)^2_j} \right] + \Theta$$

$$= \frac{\hbar^2}{4} \sum_j \lambda^2_j + \frac{\hbar^2}{4} \sum_{j'<j} \lambda_j \lambda_{j'} \left[y_{jj'} + \frac{1}{y_{jj'}} \right] + \Theta,$$

(4.17)

where the nonnegative variable

$$y_{jj'} = \frac{(\Delta x)_j^2}{(\Delta x)_{j'}^2} \tag{4.18}$$

has been defined.

Noting

$$y_{jj'} + \frac{1}{y_{jj'}} \geq 2, \quad \forall y_{jj'} \geq 0, \tag{4.19}$$

(4.17) allows to write

$$(\Delta x)^2 (\Delta v)^2 \geq \frac{\hbar^2}{4} \left[\sum_j \lambda_j^2 + 2 \sum_{j'<j} \lambda_j \lambda_{j'} \right] + \Theta = \frac{\hbar^2}{4} \left[\sum_j \lambda_j \right]^2 + \Theta. \tag{4.20}$$

Finally, remembering that for the coefficients λ_j the normalization relation holds

$$\sum_j \lambda_j = 1 \tag{4.21}$$

and that Θ is defined nonnegative, from (4.20) the following inequality is obtained:

$$\Delta x \Delta v \geq \frac{\hbar}{2} \tag{4.22}$$

which represents the Heisenberg uncertainty relation within the two-dimensional phase space $\{x, v\}$.

5. The Set of the Square-Integrable Functions: The Space S^2

Consider the set $\{f(x, v, t)\}$ constituted by the functions which obey the relation:

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv \, f(x, v, t) = 1. \tag{5.1}$$

Inside the set $\{f(x, v, t)\}$ we characterize the subset formed by the square-integrable functions, that is the functions which satisfy the following relation

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv \, |f(x, v, t)|^2 < \infty. \tag{5.2}$$

This set, named S^2, possesses the structure of a vectorial space. In fact, if we consider two arbitrary functions $f(x,v,t)$, $g(x,v,t) \in S^2$ and two arbitrary complex numbers λ_1, λ_2, for the function $\lambda_1 f(x,v,t) + \lambda_2 g(x,v,t)$ the following relation holds:

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv \left| \lambda_1 f(x,v,t) + \lambda_2 g(x,v,t) \right|^2 \leq \infty. \tag{5.3}$$

Equation (5.3) indicates that the sum of two square-integrable functions is itself a square-integrable function. The set is then closed respect to the sum. It is easy to verify the set S^2 satisfies all the properties of a vectorial space.

Moreover a *scalar product* (f,g) can be defined

$$(f,g) = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv f^*(x,v) g(x,v), \tag{5.4}$$

which associates each pair of elements of S^2 with a complex number.

The set of the functions belonging to S^2 with the scalar product defined in (5.4) constitutes a Hilbert space.

6. A Basis of S^2

In order to construct a basis of the vectorial space S^2 we consider the Hermite functions defined in (3.3). They constitute a basis of the space formed by the solutions of the Schrödinger equation. Using the generic Hermite function $S_n(x)$ it is possible to introduce the set $\{f_{nn'}(x,v)\}$ with

$$f_{nn'}(x,v) = \int_{-\infty}^{+\infty} ds\, e^{isv} e^{-(x+(\hbar/2)s)^2/2} e^{-(x-(\hbar/2)s)^2/2} \frac{H_n(x+(\hbar/2)s)}{\sqrt{\pi^{1/2}2^n n!}} \frac{H_{n'}(x-(\hbar/2)s)}{\sqrt{\pi^{1/2}2^{n'} n'!}}. \tag{6.1}$$

We propose to show that the set $\{f_{nn'}(x,v)\}$ constitutes a basis of S^2. This may be obtained by proving that $\{f_{nn'}(x,v)\}$ is an orthonormal and complete set of this space.

6.1. Orthonormality

In order to prove the orthonormality of the set $\{f_{nn'}(x,v)\}$, we calculate the following integral:

$$\begin{aligned}
&\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv\, f_{nn'}(x,v) f_{mm'}^*(x,v) \\
&\quad = \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv \int_{-\infty}^{+\infty} ds\, e^{isv} e^{-(x+(\hbar/2)s)^2/2} e^{-(x-(\hbar/2)s)^2/2} \\
&\qquad \times \frac{H_n(x+(\hbar/2)s)}{\sqrt{\pi^{1/2}2^n n!}} \frac{H_{n'}(x-(\hbar/2)s)}{\sqrt{\pi^{1/2}2^{n'} n'!}} \\
&\qquad \cdot \int_{-\infty}^{+\infty} ds'\, e^{-is'v} e^{-(x+(\hbar/2)s')^2/2} e^{-(x-(\hbar/2)s')^2/2} \frac{H_m(x+(\hbar/2)s')}{\sqrt{\pi^{1/2}2^m m!}} \frac{H_{m'}(x-(\hbar/2)s')}{\sqrt{\pi^{1/2}2^{m'} m'!}},
\end{aligned} \tag{6.2}$$

where $f_{nn'}(x,v)$, $f_{mm'}(x,v)$ are two arbitrary functions belonging to S^2. Performing the variable change

$$y = x + \frac{\hbar}{2}s, \qquad z = x - \frac{\hbar}{2}s, \tag{6.3}$$

and using the orthonormality of the Hermite functions, from (6.2) one gets

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv \, f_{nn'}(x,v) f_{mm'}^*(x,v) = 2\pi \delta_{nm} \delta_{n'm'}, \tag{6.4}$$

which represents the orthonormality relation for the functions $f_{nn'}(x,v)$.

6.2. Closure

To prove that the set $\{f_{nn'}(x,v)\}$ satisfies closure relation, we write

$$\sum_{nn'} f_{nn'}(x,v) f_{nn'}^*(x',v')$$

$$= \sum_{nn'} \int_{-\infty}^{+\infty} ds e^{\imath s v} e^{-(x+(\hbar/2)s)^2/2} e^{-(x-(\hbar/2)s)^2/2}$$

$$\times \frac{H_n(x+(\hbar/2)s)}{\sqrt{\pi^{1/2}2^n n!}} \frac{H_{n'}(x-(\hbar/2)s)}{\sqrt{\pi^{1/2}2^{n'} n'!}}$$

$$\cdot \int_{-\infty}^{+\infty} ds' e^{-\imath s' v'} e^{-(x'+(\hbar/2)s')^2/2} e^{-(x'-(\hbar/2)s')^2/2} \frac{H_n(x'+(\hbar/2)s')}{\sqrt{\pi^{1/2}2^n n!}} \frac{H_{n'}(x'-(\hbar/2)s')}{\sqrt{\pi^{1/2}2^{n'} n'!}}. \tag{6.5}$$

Applying the closure relation of the Hermite functions, from (6.5), one gets

$$\sum_{nn'} f_{nn'}(x,v) f_{nn'}^*(x',v') = 2\pi \delta(x-x') \delta(v-v'), \tag{6.6}$$

which expresses the closure relation. The set $\{f_{nn'}(x,v)\}$, which is orthonormal and complete, constitutes a basis of the space S^2.

7. Functions of the Space S^2 and Solutions of the Quantum Liouville Equation

Consider an arbitrary function $f(x,v,t) \in S^2$. Its expansion in terms of basis vectors $f_{nn'}(x,v)$ is given by

$$f(x,v,t) = \sum_{nn'} A_{nn'}(t) f_{nn'}(x,v) = \sum_{nn'} A_{nn'}(t) \int_{-\infty}^{+\infty} ds \, e^{\imath s v} S_n\left(x + \frac{\hbar}{2}s\right) S_{n'}\left(x - \frac{\hbar}{2}s\right), \tag{7.1}$$

where the coefficients $A_{nn'}(t)$ are complex numbers.

It is useful noting that (5.1) and (5.2) determine some properties of the coefficients $A_{nn'}$. In fact, using condition (5.1) in (7.1), one gets

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv \sum_{nn'} A_{nn'}(t) \int_{-\infty}^{+\infty} ds\, e^{\imath sv} S_n\left(x + \frac{\hbar}{2}s\right) S_{n'}\left(x - \frac{\hbar}{2}s\right) = 1,$$
(7.2)

which determines

$$\sum_{nn'} A_{nn'}(t) \int_{-\infty}^{+\infty} ds \int_{-\infty}^{+\infty} dv\, e^{\imath sv} \int_{-\infty}^{+\infty} dx\, S_n\left(x + \frac{\hbar}{2}s\right) S_{n'}\left(x - \frac{\hbar}{2}s\right)$$

$$= 2\pi \sum_{nn'} A_{nn'}(t) \int_{-\infty}^{+\infty} ds\, \delta(s) \int_{-\infty}^{+\infty} dx\, S_n\left(x + \frac{\hbar}{2}s\right) S_{n'}\left(x - \frac{\hbar}{2}s\right)$$
(7.3)

$$= 2\pi \sum_{nn'} A_{nn'}(t) \int_{-\infty}^{+\infty} dx\, S_n(x) S_{n'}(x) = 2\pi \sum_{nn'} A_{nn'}(t) \delta_{nn'} = 2\pi \sum_n A_{nn}(t) = 1.$$

Analogously, using (5.2) and (7.1), we get

$$\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dv\, |f(x,v,t)|^2 = 2\pi \sum_{nn'} |A_{nn'}(t)|^2 < \infty.$$
(7.4)

From (7.3) and (7.4) it results that the following conditions hold:

$$2\pi \sum_n A_{nn}(t) = 1$$

$$2\pi \sum_{nn'} |A_{nn'}(t)|^2 < \infty.$$
(7.5)

Consider again the expansion (7.1) which holds for an arbitrary function $f(x,v,t) \in S^2$. Now we introduce another hypothesis for the coefficients $A_{nn'}(t)$, that is, we suppose that the matrix $A(t) = \|A_{nn'}(t)\|$ can be put in diagonal form in L^2 (L^2 is the space which contains the square-integrable Schrödinger functions). If D is the matrix which diagonalizes $A(t)$, it results

$$D^{-1} A(t) D = A^D(t)$$
(7.6)

with

$$A_{nn'}^D(t) = \begin{cases} A_{nn}^D(t), & (n = n'), \\ 0, & (n \neq n'). \end{cases}$$
(7.7)

This transformation induces in L^2 the basis change

$$S_n(x) = DP_n(x)$$
(7.8)

where $P_n(x)$ are the vectors belonging to the new basis. The matrix elements of $\|A_{nn'}(t)\|$ represent in the space S^2 the coefficients of the expansion (7.1) on the basis vectors $\{f_{nn'}(x,v)\}$. The diagonalization defined by (7.6) induces within the space S^2 the transformation

$$f_{nn'}(x,v) \longrightarrow g_{nn'}(x,v) \tag{7.9}$$

with

$$g_{nn'}(x,v) = \int_{-\infty}^{+\infty} ds\, e^{isv} P_n\left(x + \frac{\hbar}{2}s\right) P_{n'}^*\left(x - \frac{\hbar}{2}s\right). \tag{7.10}$$

By following a procedure similar to that used for the set $\{f_{nn'}(x,v)\}$ it is easy to verify that the functions $g_{nn'}(x,v)$ satisfy relations both of ortonormality and closure. Therefore they constitute a new basis of S^2. Equation (7.1) then becomes

$$f(x,v,t) = \sum_{nn'} A_{nn'}^D(t)\delta_{nn'} g_{nn'}(x,v) = \int_{-\infty}^{+\infty} ds\, e^{isv} \sum_n \lambda_n(t)\rho_n(x,s), \tag{7.11}$$

where we set

$$\lambda_n(t) = A_{nn}^D(t),$$

$$\rho_n(x,s) = P_n\left(x + \frac{\hbar}{2}s\right) P_n^*\left(x - \frac{\hbar}{2}s\right). \tag{7.12}$$

Now we define the density matrix

$$\rho(x,s,t) = \sum_n \lambda_n(t)\rho_n(x,s). \tag{7.13}$$

Using (7.13) in (7.11) allows to write

$$f(x,v,t) = \int_{-\infty}^{+\infty} ds\, e^{isv}\rho(x,s,t). \tag{7.14}$$

Equation (7.14) indicates that any function $f(x,v,t) \in S^2$, whose matrix $\|A_{nn'}(t)\|$ is diagonalizable, may be expressed as Fourier transform of a density matrix and then it verifies the Heisenberg uncertainty relation given in (4.22).

8. Conclusions

The quantum Liouville equation allows to deal with a quantum system using methods and tools of the statistic mechanics. This equation is derived from a typical quantum equation, that is the Schrödinger equation. In order to characterize the set of solutions of the quantum

Liouville equation which satisfy the Heisenberg uncertainty principle we investigated both the Schrödinger equation and the quantum Liouville equation. So, we recalled that an arbitrary solution $\psi(x)$ of the Schrödinger equation, because of its expansibility in plane waves,

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk\, \overline{\psi}(k) e^{\iota k x}, \tag{8.1}$$

verifies the inequality

$$\Delta \widehat{X} \Delta \widehat{P} \geq \frac{\hbar}{2}, \tag{8.2}$$

where $\widehat{X}$ and $\widehat{P}$ are observables which satisfy the commutation rule

$$\left[\widehat{X}, \widehat{P}\right] = \iota \hbar. \tag{8.3}$$

Afterwards we investigated the Heisenberg inequality with reference to the quantum Liouville equation. We studied three different cases. Initially a particular solution of the quantum Liouville equation has been considered, this solution being the Wigner transform $f(x, v, t)$ of an arbitrary wave function $\psi(x, t)$. So, we found that the product of the variances Δx and Δv, which are defined within a two-dimensional phase space, verifies the Heisenberg uncertainty relation. Then we considered a more general case: the quantum Liouville equation has been resolved by using the Fourier transform of the density matrix of an arbitrary quantum state. This allows to deal with states which cannot be represented by a wave function. The expressions obtained for the variances Δx and Δv verify the Heisenberg relation and allow to extend the result obtained for the pure state case to the statistical mixture of states. Finally, we showed that an arbitrary function $f(x, v, t) \in S^2$ admits the following expansion:

$$f(x, v, t) = \sum_{nn'} A_{nn'}(t) \int_{-\infty}^{+\infty} ds\, e^{\iota s v} S_n\left(x + \frac{\hbar}{2} s\right) S_{n'}\left(x - \frac{\hbar}{2} s\right), \tag{8.4}$$

and this expression can be written as Fourier transform of a density matrix provided that the matrix $\|A_{nn'}(t)\|$ is diagonalizable.

In conclusion we applied an alternative procedure, based on the use of the Hermite functions, to characterize the solutions of the quantum Liouville equation which verify the Heisenberg uncertainty relation.

Acknowledgments

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